

```

C *****
C * PDE2D 9.2 MAIN PROGRAM *
C *****
C *** 2D PROBLEM SOLVED (COLLOCATION METHOD) ***
C#####
C Is double precision mode to be used? Double precision is recommended #
C on 32-bit computers. #
C #
C ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C + If double precision mode is used, variables and functions assigned + #
C + names beginning with a letter in the range A-H or O-Z will be DOUBLE + #
C + PRECISION, and you should use double precision constants and FORTRAN + #
C + expressions throughout; otherwise such variables and functions will + #
C + be of type REAL. In either case, variables and functions assigned + #
C + names beginning with I,J,K,L,M or N will be of INTEGER type. + #
C + #
C + It is possible to convert a single precision PDE2D program to double + #
C + precision after it has been created, using an editor. Just change + #
C + all occurrences of "real" to "double precision" + #
C + " tdp" to "dtdp" (note leading blank) + #
C + Any user-written code or routines must be converted "by hand", of + #
C + course. To convert from double to single, reverse the changes. + #
C ++++++ END OF "FINE PRINT" ++++++ #
C#####
C implicit double precision (a-h,o-z)
C parameter (neqnm= 99)
C#####
C NP1GRID = number of P1-grid lines #
C#####
C-----> INPUT FROM GUI <-----
C PARAMETER (NP1GRID = 18)
C#####
C NP2GRID = number of P2-grid lines #
C#####
C-----> INPUT FROM GUI <-----
C PARAMETER (NP2GRID = 16)
C#####
C How many differential equations (NEQN) are there in your problem? #
C#####
C PARAMETER (NEQN = 4)
C parameter (np3grid = 1)
C DIMENSIONS OF WORK ARRAYS
C SET TO 1 FOR AUTOMATIC ALLOCATION
C PARAMETER (IRWK8Z= 1)
C PARAMETER (IIWK8Z= 1)
C PARAMETER (NXP8Z=101,NYP8Z=101,KDEG8Z=1,NZP8Z=KDEG8Z+1)
C#####
C The solution is normally saved on an NP1+1 by NP2+1 rectangular grid #
C of points, #
C P1 = P1A + I*(P1B-P1A)/NP1, I = 0,...,NP1 #
C P2 = P2A + J*(P2B-P2A)/NP2, J = 0,...,NP2 #
C Enter values for NP1 and NP2. Suggested values: NP1=NP2=25. #
C #
C ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C + If you want to save the solution at an arbitrary user-specified set + #
C + of points, set NP2=0 and NP1+1=number of points. In this case you + #
C + can request tabular output, but no plots can be made. + #
C + #
C + If you set NEAR8Z=1 in the main program, the values saved at each + #
C + output point will actually be the solution as evaluated at a nearby + #
C + collocation point. For most problems this obviously will produce + #
C + less accurate output or plots, but for certain (rare) problems, a + #
C + solution component may be much less noisy when plotted only at + #
C + collocation points. + #

```

```

C      ++++++ END OF "FINE PRINT" ++++++#
C#####
C      PARAMETER (NP1 = 140)
C      PARAMETER (NP2 = 63)
C#####
C      The solution will be saved (for possible postprocessing) at the NSAVE+1 #
C      time points #
C      T0 + K*(TF-T0)/NSAVE #
C      K=0,...,NSAVE. Enter a value for NSAVE. #
C #
C      If a user-specified constant time step is used, NSTEPS must be an #
C      integer multiple of NSAVE. #
C#####
C      PARAMETER (NSAVE =150)
C      common/parm8z/pi,DCA,Umax,EC50 ,Hill,CArest,RC,Aca
C      &,OD2,Slope ,Slope2,Width,TN,Flu,Cal,ktn_p,ktn_n,kcal_p
C      &,kflu_n,Dcal,Dflu ,DU ,OTB ,kcal_n, kflu_p
C      dimension plgrid(np1grid),p2grid(np2grid),p3grid(np3grid),plout8z(
C      &0:np1,0:np2),p2out8z(0:np1,0:np2),p3out8z(0:np1,0:np2),plcross(100
C      &),p2cross(100),tout8z(0:nsave),uout8z(0:np1,0:np2,4*neqn,0:nsave),
C      &uout(0:np1,0:np2,4,neqn,0:nsave),xres8z(nxp8z),yres8z(nyp8z),zres8
C      &z(nzp8z),ures8z(neqn,nxp8z,nyp8z,nzp8z)
C      equivalence (uout,uout8z)
C      allocatable iwrk8z(:),rwrk8z(:)
C      dimension iwrk8z(iiwk8z),rwrk8z(irwk8z)
C      character*40 title
C      logical linear,crankn,noupdt,nodist,fillin,evcmpx,adapt,plot,lsqfi
C      &t,fdiff,solid,econ8z,ncon8z,resttr,gridid
C      common/dtdp14/ sint8z(20),bint8z(20),slim8z(20),blim8z(20)
C      common/dtdp15/ evlr8z,ev0r,evli8z,ev0i,evcmpx
C      common/dtdp16/ p8z,evr8z(50),evi8z(50)
C      common/dtdp19/ toler(neqnm),adapt
C      common/dtdp30/ econ8z,ncon8z
C      common/dtdp45/ perdc(neqnm)
C      common/dtdp46/ eps8z,cgtl8z,npmx8z,itype,near8z
C      common/dtdp52/ nxa8z,nya8z,nza8z,kd8z
C      common/dtdp53/ work8z(nxp8z*nyp8z*nzp8z+9)
C      common/dtdp64/ amin8z(4*neqnm),amax8z(4*neqnm)
C      pi = 4.0*atan(1.d0)
C      zr8z = 0.0
C      nxa8z = nxp8z
C      nya8z = nyp8z
C      nza8z = nzp8z
C      kd8z = kdeg8z
C#####
C      If you don't want to read the FINE PRINT, default NPROB. #
C #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#
C      + If you want to solve several similar problems in the same run, set + #
C      + NPROB equal to the number of problems you want to solve. Then NPROB + #
C      + loops through the main program will be done, with IPROB=1,...,NPROB, + #
C      + and you can make the problem parameters vary with IPROB. NPROB + #
C      + defaults to 1. + #
C      ++++++ END OF "FINE PRINT" ++++++#
C#####
C      NPROB = 1
C      do 78755 iprob=1,nprob
C#####
C      You may now define global parameters, which may be referenced in any #
C      of the "FORTRAN expressions" you input throughout the rest of this #
C      interactive session. You will be prompted alternately for parameter #

```

```

C      names and their values; enter a blank name when you are finished.      #
C                                                                              #
C      Parameter names are valid FORTRAN variable names, starting in        #
C      column 1.  Thus each name consists of 1 to 6 alphanumeric characters,  #
C      the first of which must be a letter.  If the first letter is in the   #
C      range I-N, the parameter must be an integer.                          #
C                                                                              #
C      Parameter values are either FORTRAN constants or FORTRAN expressions  #
C      involving only constants and global parameters defined on earlier     #
C      lines.  They may also be functions of the problem number IPROB, if    #
C      you are solving several similar problems in one run (NPROB > 1).  Note #
C      that you are defining global CONSTANTS, not functions; e.g., parameter #
C      values may not reference any of the independent or dependent variables #
C      of your problem.                                                       #
C                                                                              #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++              #
C      + If you define other parameters here later, using an editor, you must + #
C      + add them to COMMON block /PARM8Z/ everywhere this block appears, if + #
C      + they are to be "global" parameters.                                + #
C      +                                                                 + #
C      + The variable PI is already included as a global parameter, with an + #
C      + accurate value 3.14159...                                         + #
C      ++++++ END OF "FINE PRINT" ++++++                                    #
C#####
C-----> INPUT FROM GUI <-----
C----- Diffusion coefficient of Calcium ion -----
      Umax      =
      & 200
C----- Median effective Ca2+ concentration -----
      EC50      =
      & 0.2
C----- Hill coefficient -----
      Hill      =
      & 2
C----- diffusion coefficients for Ca2+ ---
      DCA       =
      & 600
C----- Resting Calcium Concentration -----
      CArest    =
      & 0.1
C----- rate constant of activation -----
      RC        =
      & 2
C-----maximum amplitude of Ca2+ flux-----
      Aca       =
      & 180
C----- variable time offset -----
      DU        =
      & 0
C----- Time base -----
      OTB       =
      & 100
C----- Slope1-----
      Slope     =
      & 44
C----- Slope2 -----
      Slope2    =
      & 0.06*Slope
C----- release pulse modulator -----
      Pulse     =
      & 40
C----- Deactivating time constant -----
      OD2       =

```

```

    & OTB*Slope/Pulse
C----- Troponin C Concentration -----
    TN      =
    & 40
C----- Fluo-4 concentration -----
    Flu     =
    & 100
C----- Calmodulin Concentration -----
    Cal     =
    & 24
C----- On rate of Ca2+-Troponin C-----
    ktn_p   =
    & 39
C----- Off rate of Ca2+-Troponin C -----
    ktn_n   =
    & 20
C-----On rate Ca2+-Calmodulin -----
    kcal_p  =
    & 125
C----- Off rate Ca2+-Calmodulin -----
    kcal_n  =
    & 297.5
C----- On rate Ca2+-Fluo-4 -----
    kflu_p  =
    & 230
C-----Off rate Ca2+-Fluo-4 -----
    kflu_n  =
    & 170
C----- diffusion coefficients for Ca-CaM -----
    DCal    =
    & 25
C----- diffusion coefficients for Ca-Flou4 -----
    Dflu    =
    & 100

C#####
C    A collocation finite element method is used, with bi-cubic Hermite #
C    basis functions on the elements (small rectangles) defined by the grid #
C    points: #
C          P1GRID(1),...,P1GRID(NP1GRID) #
C          P2GRID(1),...,P2GRID(NP2GRID) #
C    You will first be prompted for NP1GRID, the number of P1-grid points, #
C    then for P1GRID(1),...,P1GRID(NP1GRID). Any points defaulted will be #
C    uniformly spaced between the points you define; the first and last #
C    points cannot be defaulted. Then you will be prompted similarly #
C    for the number and values of the P2-grid points. The limits on the #
C    parameters are then: #
C          P1GRID(1) < P1 < P1GRID(NP1GRID) #
C          P2GRID(1) < P2 < P2GRID(NP2GRID) #
C #
C#####
C          call dtdpwx(plgrid,np1grid,0)
C          call dtdpwx(p2grid,np2grid,0)
C          P1GRID DEFINED
C-----> INPUT FROM GUI <-----
C          P1GRID(1) =
C          & 0

C-----> INPUT FROM GUI <-----
C          P1GRID(NP1GRID) =
C          & 30
C          P2GRID DEFINED

```

```

C-----> INPUT FROM GUI <-----
      P2GRID(1) =
      & 0

C-----> INPUT FROM GUI <-----
      P2GRID(NP2GRID) =
      & 12

C
      p3grid(1) = 0
      call dtdpwx(plgrid,np1grid,1)
      call dtdpwx(p2grid,np2grid,1)
C#####
C      If you don't want to read the FINE PRINT, enter ISOLVE = 1.      #
C      #                                                                    #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++          #
C      + The following linear system solvers are available:              +#+
C      +                                                                    +#+
C      + 1. Sparse direct method                                          +#+
C      +           Harwell Library routine MA27 (used by permission) is  +#+
C      +           used to solve the (positive definite) "normal"       +#+
C      +           equations  $A^T A x = A^T b$ . The normal equations,    +#+
C      +           which are essentially the equations which would result +#+
C      +           if a least squares finite element method were used    +#+
C      +           instead of a collocation method, are substantially    +#+
C      +           more ill-conditioned than the original system  $Ax = b$ ,  +#+
C      +           so it may be important to use high precision if this  +#+
C      +           option is chosen.                                       +#+
C      + 2. Frontal method                                                +#+
C      +           This is an out-of-core band solver. If you want to    +#+
C      +           override the default number of rows in the buffer (11), +#+
C      +           set a new value for NPMX8Z in the main program.        +#+
C      + 3. Jacobi conjugate gradient iterative method                    +#+
C      +           A preconditioned conjugate gradient iterative method   +#+
C      +           is used to solve the (positive definite) normal       +#+
C      +           equations. High precision is also important if this    +#+
C      +           option is chosen. (This solver is MPI-enhanced, if     +#+
C      +           MPI is available.) If you want to override the        +#+
C      +           default convergence tolerance, set a new relative      +#+
C      +           tolerance CGTL8Z in the main program.                  +#+
C      + 4. Local solver (normal equations)                               +#+
C      + 5. Local solver (original equations)                             +#+
C      +           Choose these options ONLY if alternative linear system  +#+
C      +           solvers have been installed locally. See subroutines   +#+
C      +           (D)TD3M, (D)TD3N in file (d)subs.f for instructions    +#+
C      +           on how to add local solvers.                           +#+
C      + 6. MPI-based parallel band solver                                +#+
C      +           This is a parallel solver which runs efficiently on    +#+
C      +           multiple processor machines, under MPI. It is a        +#+
C      +           band solver, with the matrix distributed over the      +#+
C      +           available processors. Choose this option ONLY if the   +#+
C      +           solver has been activated locally. See subroutine      +#+
C      +           (D)TD30 in file (d)subs.f for instructions on how to   +#+
C      +           activate this solver and the MPI-enhancements to the   +#+
C      +           conjugate gradient solver.                               +#+
C      +           #                                                                    +#+
C      + Enter ISOLVE = 1,2,3,4,5 or 6 to select a linear system solver.  +#+
C      ++++++ END OF "FINE PRINT" ++++++          #
C#####
C      ISOLVE =      2
C      *****TIME-DEPENDENT PROBLEM
C      itype = 2
C#####
C      Enter the initial time value (T0) and the final time value (TF), for #
C      this time-dependent problem. T0 defaults to 0.                      #

```

```

C                                                                 #
C   TF is not required to be greater than T0.                    #
C#####
C   T0 = 0.0
C-----> INPUT FROM GUI <-----
C   T0 =
C   & 0
C-----> INPUT FROM GUI <-----
C   TF =
C   & 0.3
C#####
C   Is this a linear problem? ("linear" means all differential equations #
C   and all boundary conditions are linear).  If you aren't sure, it is #
C   safer to answer "no".                                         #
C#####
C   LINEAR = .FALSE.
C#####
C   Do you want the time step to be chosen adaptively?  If you answer #
C   'yes', you will then be prompted to enter a value for TOLER(1), the #
C   local relative time discretization error tolerance.  The default is #
C   TOLER(1)=0.01.  If you answer 'no', a user-specified constant time step #
C   will be used.  We suggest that you answer 'yes' and default TOLER(1) #
C   (although for certain linear problems, a constant time step may be much #
C   more efficient).
C   #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++
C   + If a negative value is specified for TOLER(1), then ABS(TOLER(1)) is +
C   + taken to be the "absolute" error tolerance.  If a system of PDEs is +
C   + solved, by default the error tolerance specified in TOLER(1) applies +
C   + to all variables, but the error tolerance for the J-th variable can +
C   + be set individually by specifying a value for TOLER(J) using an +
C   + editor, after the end of the interactive session.             +
C   +
C   + Each time step, two steps of size dt/2 are taken, and that solution +
C   + is compared with the result when one step of size dt is taken.  If +
C   + the maximum difference between the two answers is less than the +
C   + tolerance (for each variable), the time step dt is accepted (and the +
C   + next step dt is doubled, if the agreement is "too" good); otherwise +
C   + dt is halved and the process is repeated.  Note that forcing the +
C   + local (one-step) error to be less than the tolerance does not +
C   + guarantee that the global (cumulative) error is less than that value.+
C   + However, as the tolerance is decreased, the global error should +
C   + decrease correspondingly.
C   ++++++ END OF "FINE PRINT" ++++++
C#####
C-----> INPUT FROM GUI <-----
C   ADAPT = .FALSE.
C   TOLER(1) = 0.001
C   TOLER(1) =
C   & 0.05
C   NOUPDT = .FALSE.
C#####
C   The time stepsize will be chosen adaptively, between an upper limit #
C   of DTMAX = (TF-T0)/NSTEPS and a lower limit of 0.0001*DTMAX.  Enter #
C   a value for NSTEPS (the minimum number of steps).             #
C   #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++
C   + If you later turn off adaptive time step control, the time stepsize +
C   + will be constant, DT = (TF-T0)/NSTEPS.                       +
C   ++++++ END OF "FINE PRINT" ++++++
C#####
C-----> INPUT FROM GUI <-----
C   NSTEPS =
C   & 300

```

```

dt = (tf-t0)/max(nsteps,1)
C#####
C   If you don't want to read the FINE PRINT, enter 'no'.           #
C   #                                                                 #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++      #
C   + Is the Crank-Nicolson scheme to be used to discretize time? If you + #
C   + answer 'no', a backward Euler scheme will be used.          + #
C   +                                                                 + #
C   + If a user-specified constant time step is chosen, the second order + #
C   + Crank Nicolson method is recommended only for problems with very + #
C   + well-behaved solutions, and the first order backward Euler scheme + #
C   + should be used for more difficult problems. In particular, do not + #
C   + use the Crank Nicolson method if the left hand side of any PDE is + #
C   + zero, for example, if a mixed elliptic/parabolic problem is solved. + #
C   +                                                                 + #
C   + If adaptive time step control is chosen, however, an extrapolation + #
C   + is done between the 1-step and 2-step answers which makes the Euler + #
C   + method second order, and the Crank-Nicolson method strongly stable. + #
C   + Thus in this case, both methods have second order accuracy, and both + #
C   + are strongly stable.                                         + #
C   ++++++ END OF "FINE PRINT" ++++++                              #
C#####
C   CRANKN = .FALSE.
C   FDIFF = .TRUE.
C#####
C   You may calculate one or more integrals (over the entire region) of #
C   some functions of the solution and its derivatives. How many integrals #
C   (NINT), if any, do you want to calculate?                       #
C   #                                                                 #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++      #
C   + In the FORTRAN program created by the preprocessor, the computed + #
C   + values of the integrals will be returned in the vector SINT8Z. If + #
C   + several iterations or time steps are done, only the last computed + #
C   + values are saved in SINT8Z (all values are printed).          + #
C   +                                                                 + #
C   + A limiting value, SLIM8Z(I), for the I-th integral can be set + #
C   + below in the main program. The computations will then stop + #
C   + gracefully whenever SINT8Z(I) > SLIM8Z(I), for any I=1..NINT. + #
C   ++++++ END OF "FINE PRINT" ++++++                              #
C#####
C-----> INPUT FROM GUI <-----
NINT = 0
C#####
C   You may calculate one or more boundary integrals (over the entire #
C   boundary) of some functions of the solution and its derivatives. How #
C   many boundary integrals (NBINT), if any, do you want to calculate? #
C   #                                                                 #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++      #
C   + In the FORTRAN program created by the preprocessor, the computed + #
C   + values of the integrals will be returned in the vector BINT8Z. If + #
C   + several iterations or time steps are done, only the last computed + #
C   + values are saved in BINT8Z (all values are printed).          + #
C   +                                                                 + #
C   + A limiting value, BLIM8Z(I), for the I-th boundary integral can be + #
C   + set below in the main program. The computations will then stop + #
C   + gracefully whenever BINT8Z(I) > BLIM8Z(I), for any I=1..NBINT. + #
C   ++++++ END OF "FINE PRINT" ++++++                              #
C#####
C   NBINT = 0
C#####
C   If you don't want to read the FINE PRINT, enter 'no'.           #
C   #                                                                 #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++      #
C   + Normally, interpolation is done to approximate the initial values + #

```

```

C      + using cubic Hermites.  Since some derivatives must be interpolated,  + #
C      + if the initial values are not smooth (ie, have large or infinite    + #
C      + derivatives), the resulting cubic interpolants may have undesired    + #
C      + noise or large spikes.  Do you want to compute a least squares      + #
C      + approximation to the initial values, rather than an interpolant?    + #
C      + The least squares fit is generally much smoother, but requires one   + #
C      + extra linear system solution.                                       + #
C      ++++++ END OF "FINE PRINT" ++++++                                     + #
C#####
C      LSQFIT = .FALSE.
C#####
C      If you don't want to read the FINE PRINT, enter 'no'.                + #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++             + #
C      + Do you want to read the initial conditions from the restart file,    + #
C      + if it exists (and use the conditions supplied above if it does not  + #
C      + exist)?                                                                + #
C      + ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++             + #
C      + If so, PDE2D will dump the final solution at the end of each run    + #
C      + into a restart file "pde2d.res".  Thus the usual procedure for      + #
C      + using this dump/restart option is to make sure there is no restart  + #
C      + file in your directory left over from a previous job, then the     + #
C      + first time you run this job, the initial conditions supplied above  + #
C      + will be used, but on the second and subsequent runs the restart file + #
C      + from the previous run will be used to define the initial conditions. + #
C      + ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++             + #
C      + You can do all the "runs" in one program, by setting NPROB > 1.    + #
C      + Each pass through the DO loop, T0,TF,NSTEPS and possibly other      + #
C      + parameters may be varied, by making them functions of IPROB.       + #
C      + ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++             + #
C      + If the 2D or 3D collocation method is used, the coordinate          + #
C      + transformation should not change between dump and restart.          + #
C      ++++++ END OF "FINE PRINT" ++++++                                     + #
C#####
C      RESTRT = .FALSE.
C      GRIDID = .FALSE. IF FINITE ELEMENT GRID CHANGES BETWEEN DUMP, RESTART
C      GRIDID = .TRUE.
C#####
C      If you do not have any periodic boundary conditions, enter IPERDC=0.  + #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++             + #
C      Enter IPERDC=1 for periodic conditions at P1 = P1GRID(1),P1GRID(NP1GRID) + #
C      IPERDC=2 for periodic conditions at P2 = P2GRID(1),P2GRID(NP2GRID)    + #
C      IPERDC=4 for periodic conditions on both P1 and P2                     + #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++             + #
C      + When periodic boundary conditions are selected, they apply to all    + #
C      + variables by default.  To turn off periodic boundary conditions on  + #
C      + the I-th variable, set PERDC(I) to 0 (or another appropriate value  + #
C      + of IPERDC) below in the main program and set the desired boundary  + #
C      + conditions in subroutine GB8Z, "by hand".                            + #
C      ++++++ END OF "FINE PRINT" ++++++                                     + #
C#####
C-----> INPUT FROM GUI <-----
C      IPERDC =          0
C#####
C      The solution is saved on an NP1+1 by NP2+1 rectangular grid covering  + #
C      the rectangle (P1A,P1B) x (P2A,P2B).  Enter values for P1A,P1B,P2A,P2B. + #
C      These variables are usually defaulted.                                  + #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++             + #
C      The defaults are P1A = P1GRID(1), P1B = P1GRID(NP1GRID)              + #
C      P2A = P2GRID(1), P2B = P2GRID(NP2GRID)                                + #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++             + #
C#####
C      defaults for pla,p1b,p2a,p2b
C      pla = plgrid(1)

```



```

p1b = p1grid(np1grid)
p2a = p2grid(1)
p2b = p2grid(np2grid)
C   DEFINE P1A,P1B,P2A,P2B HERE:
call dtdpx3(np1,np2,0,p1a,p1b,p2a,p2b,zr8z,zr8z,hp18z,hp28z,hp38z,
&plout8z,p2out8z,p3out8z,npts8z)
C   *****allocate workspace
call dtdpqx(np1grid,np2grid,np3grid,ISOLVE,NEQN,II8Z,IR8Z,IPERDC)
if (iiwk8z.gt.1) ii8z = iiwk8z
if (irwk8z.gt.1) ir8z = irwk8z
allocate (iwrk8z(ii8z),rwrk8z(ir8z))
C   *****DRAW GRID LINES?
PLOT = .TRUE.
C   *****call pde solver
call dtdp3x(p1grid, p2grid, p3grid, np1grid,np2grid, -1, neqn, plo
&ut8z, p2out8z, p3out8z, uout, tout8z, npts8z, t0, dt, nsteps, nout
&, nsave, crankn, noupdt, itype, linear, ISOLVE, rwrk8z, ir8z, iwrk
&8z, ii8z, iperdc, plot, lsqfit, fdiff, nint, nbint, restrt, gridid
&)
deallocate (iwrk8z,rwrk8z)
C   *****read from restart file to array ures8z
call dtdpr3(1,xres8z,nxp8z,yres8z,nyp8z,zres8z,nzp8z,ures8z,neqn)
C   *****write array ures8z back to restart file
call dtdpr3(2,xres8z,nxp8z,yres8z,nyp8z,zres8z,nzp8z,ures8z,neqn)
C   *****call user-written postprocessor
call postpr(tout8z,nsave,plout8z,p2out8z,np1,np2,uout,neqn)
C   *****CONTOUR PLOTS
C#####
C   Enter a value for IVAR, to select the variable to be plotted or      #
C   printed:                                                             #
C       IVAR = 1 means Ca (possibly as modified by UPRINT,..)          #
C           2      Cax                                                  #
C           3      Cay                                                  #
C           4      CaT                                                  #
C           5      CaTx                                                 #
C           6      CaTy                                                 #
C           7      CaC                                                  #
C           8      CaCx                                                 #
C           9      CaCy                                                 #
C          10     CaF                                                  #
C          11     CaFx                                                  #
C          12     CaFy                                                  #
C           .      .                                                  #
C           .      .                                                  #
C#####
C       IVAR = 1
C#####
C   If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC. #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++          #
C   + The tabular output or plots will be made at times:              + #
C   +       T(K) = T0 + K*(TF-T0)/NSAVE                               + #
C   + for     K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2        + #
C   + Enter values for ISET1, ISET2 and ISINC.                         + #
C   +                                                                 + #
C   + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular + #
C   + output or plots will be made at all time values for which the   + #
C   + solution has been saved.                                         + #
C   ++++++ END OF "FINE PRINT" ++++++                                  #
C#####
C       ISET1 = 0
C       ISET2 = NSAVE
C       ISINC = 1
C#####

```



```

C                                     .       .                               #
C                                     .       .                               #
C#####
C      IVAR =          4
C#####
C      If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC.      #
C                                     #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C      + The tabular output or plots will be made at times:                + #
C      +      T(K) = T0 + K*(TF-T0)/NSAVE                                  + #
C      + for      K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2          + #
C      + Enter values for ISET1, ISET2 and ISINC.                          + #
C      +                                                                     + #
C      + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular  + #
C      + output or plots will be made at all time values for which the     + #
C      + solution has been saved.                                          + #
C      ++++++ END OF "FINE PRINT" ++++++ #
C#####
C      ISET1 = 0
C      ISET2 = NSAVE
C      ISINC = 1
C#####
C      If you don't want to read the FINE PRINT, enter 'no'.                #
C                                     #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C      + Do you want to scale the axes on the plot so that the region is    + #
C      + undistorted? Otherwise the axes will be scaled so that the figure  + #
C      + approximately fills the plot space.                                + #
C      ++++++ END OF "FINE PRINT" ++++++ #
C#####
C      NODIST = .FALSE.
C
C      ivar8z = ivar + (ivar-1)/3
C      alow = amin8z(ivar8z)
C      ahigh = amax8z(ivar8z)
C#####
C      Enter lower (UMIN) and upper (UMAX) bounds for the contour values. UMIN #
C      and UMAX are often defaulted.                                         #
C                                     #
C      Labeled contours will be drawn corresponding to the values            #
C                                     #
C      UMIN + S*(UMAX-UMIN),      for S=0.05,0.15,...0.95.                #
C                                     #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C      + By default, UMIN and UMAX are set to the minimum and maximum values + #
C      + of the variable to be plotted. For a common scaling, you may want  + #
C      + to set UMIN=ALOW, UMAX=AHIGH. ALOW and AHIGH are the minimum and   + #
C      + maximum values over all output points and over all saved time steps + #
C      + or iterations.                                                    + #
C      ++++++ END OF "FINE PRINT" ++++++ #
C#####
C      UMIN = alow
C      UMAX = ahigh
C#####
C      Do you want two additional unlabeled contours to be drawn between each #
C      pair of labeled contours?                                             #
C#####
C      FILLIN = .TRUE.
C#####
C      Enter a title, WITHOUT quotation marks. A maximum of 40 characters    #
C      are allowed. The default is no title.                                #
C#####
C      TITLE = ' '
C      TITLE = 'CaT

```

```

call dtdprx(tout8z,nsave,iset1,iset2,isinc)
do 78757 is8z=iset1,iset2,isinc
call dtdpln(uout8z(0,0,ivar8z,is8z),np1,np2,0,p1a,p1b,p2a,p2b,zr8z
&,zr8z,3,ix8z,jy8z,0,title,umin,umax,nodist,fillin,tout8z(is8z),zr8
&z,zr8z,zr8z,zr8z,2,ical8z)
78757 continue
C      *****CONTOUR PLOTS
C#####
C      Enter a value for IVAR, to select the variable to be plotted or      #
C      printed:                                                              #
C          IVAR = 1 means Ca (possibly as modified by UPRINT,..)          #
C              2      Cax                                                  #
C              3      Cay                                                  #
C              4      CaT                                                  #
C              5      CaTx                                                 #
C              6      CaTy                                                 #
C              7      CaC                                                  #
C              8      CaCx                                                 #
C              9      CaCy                                                 #
C             10      CaF                                                  #
C             11      CaFx                                                 #
C             12      CaFy                                                 #
C              .      .                                                  #
C              .      .                                                  #
C#####
C          IVAR =          7
C#####
C      If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC.  #
C      #                                                                    #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++            #
C      + The tabular output or plots will be made at times:                + #
C      +      T(K) = T0 + K*(TF-T0)/NSAVE                                  + #
C      + for      K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2        + #
C      + Enter values for ISET1, ISET2 and ISINC.                          + #
C      +                                                                    + #
C      + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular + #
C      + output or plots will be made at all time values for which the    + #
C      + solution has been saved.                                          + #
C      ++++++ END OF "FINE PRINT" ++++++
C#####
C          ISET1 = 0
C          ISET2 = NSAVE
C          ISINC = 1
C#####
C      If you don't want to read the FINE PRINT, enter 'no'.              #
C      #                                                                    #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++            #
C      + Do you want to scale the axes on the plot so that the region is    + #
C      + undistorted? Otherwise the axes will be scaled so that the figure + #
C      + approximately fills the plot space.                                + #
C      ++++++ END OF "FINE PRINT" ++++++
C#####
C          NODIST = .FALSE.
C
C          ivar8z = ivar + (ivar-1)/3
C          alow = amin8z(ivar8z)
C          ahigh = amax8z(ivar8z)
C#####
C      Enter lower (UMIN) and upper (UMAX) bounds for the contour values. UMIN #
C      and UMAX are often defaulted.                                       #
C      #                                                                    #
C      Labeled contours will be drawn corresponding to the values          #
C      #                                                                    #
C          UMIN + S*(UMAX-UMIN),      for S=0.05,0.15,...0.95.          #

```

```

C                                                                 #
C ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C + By default, UMIN and UMAX are set to the minimum and maximum values + #
C + of the variable to be plotted. For a common scaling, you may want + #
C + to set UMIN=ALOW, UMAX=AHIGH. ALOW and AHIGH are the minimum and + #
C + maximum values over all output points and over all saved time steps + #
C + or iterations. + #
C ++++++ END OF "FINE PRINT" ++++++ #
C#####
C      UMIN = aLOW
C      UMAX = aHIGH
C#####
C      Do you want two additional unlabeled contours to be drawn between each #
C      pair of labeled contours? #
C#####
C      FILLIN = .TRUE.
C#####
C      Enter a title, WITHOUT quotation marks. A maximum of 40 characters #
C      are allowed. The default is no title. #
C#####
C      TITLE = ' '
C      TITLE = 'CaC'
C      call dtdprx(tout8z,nsave,iset1,iset2,isinc)
C      do 78758 is8z=iset1,iset2,isinc
C      call dtdpln(uout8z(0,0,ivar8z,is8z),np1,np2,0,p1a,p1b,p2a,p2b,zr8z
C      &,zr8z,3,ix8z,jy8z,0,title,umin,umax,nodist,fillin,tout8z(is8z),zr8
C      &z,zr8z,zr8z,zr8z,2,ical8z)
78758 continue
C      *****CONTOUR PLOTS
C#####
C      Enter a value for IVAR, to select the variable to be plotted or #
C      printed: #
C      IVAR = 1 means Ca (possibly as modified by UPRINT,..) #
C      2      Cax #
C      3      Cay #
C      4      CaT #
C      5      CaTx #
C      6      CaTy #
C      7      CaC #
C      8      CaCx #
C      9      CaCy #
C      10     CaF #
C      11     CaFx #
C      12     CaFy #
C      .      . #
C      .      . #
C#####
C      IVAR =      10
C#####
C      If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC. #
C      #
C ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C + The tabular output or plots will be made at times: + #
C +      T(K) = T0 + K*(TF-T0)/NSAVE + #
C + for      K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2 + #
C + Enter values for ISET1, ISET2 and ISINC. + #
C + + #
C + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular + #
C + output or plots will be made at all time values for which the + #
C + solution has been saved. + #
C ++++++ END OF "FINE PRINT" ++++++ #
C#####
C      ISET1 = 0
C      ISET2 = NSAVE

```



```

C          11          CaFx          #
C          12          CaFy          #
C          .           .           #
C          .           .           #
C#####
C          IVAR =          1
C#####
C          If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC.      #
C          #
C          ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++
C          + The tabular output or plots will be made at times:                      +#
C          +          T(K) = T0 + K*(TF-T0)/NSAVE                                  +#
C          + for          K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2          +#
C          + Enter values for ISET1, ISET2 and ISINC.                              +#
C          +          #
C          + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular    +#
C          + output or plots will be made at all time values for which the        +#
C          + solution has been saved.                                             +#
C          ++++++ END OF "FINE PRINT" ++++++
C#####
C          ISET1 = 0
C          ISET2 = NSAVE
C          ISINC = 1
C#####
C          Enter the view latitude, VLAT, and the view longitude, VLON, desired      #
C          for this plot, in degrees. VLAT and VLON must be between 10 and 80      #
C          degrees; each defaults to 45 degrees. VLAT and VLON are usually        #
C          defaulted.                                                              #
C#####
C          VLON = 45.0
C          VLAT = 45.0
C
C          ivar8z = ivar + (ivar-1)/3
C          alow = amin8z(ivar8z)
C          ahigh = amax8z(ivar8z)
C#####
C          Specify the range (UMIN,UMAX) for the dependent variable axis. UMIN      #
C          and UMAX are often defaulted.                                          #
C          #
C          ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++
C          + By default, each plot will be scaled to just fit in the plot area.    +#
C          + For a common scaling, you may want to set UMIN=ALOW, UMAX=AHIGH.      +#
C          + ALOW and AHIGH are the minimum and maximum values over all output    +#
C          + points and over all saved time steps or iterations.                  +#
C          ++++++ END OF "FINE PRINT" ++++++
C#####
C          UMIN = 0.0
C          UMAX = 0.0
C          UMIN =
C          & alow
C          UMAX =
C          & ahigh
C#####
C          Enter a title, WITHOUT quotation marks. A maximum of 40 characters      #
C          are allowed. The default is no title.                                  #
C#####
C          TITLE = ' '
C          TITLE = 'Ca '
C          call dtdprx(tout8z,nsave,iset1,iset2,isinc)
C          do 78760 is8z=iset1,iset2,isinc
C          call dtdplo(plout8z,p2out8z,p3out8z,uout8z(0,0,ivar8z,is8z),np1,np
C          &2,0,3,ix8z,jy8z,0,title,vlon,vlat,umin,umax,tout8z(is8z))
78760 continue
C          *****SURFACE PLOTS

```





```

& ahigh
C#####
C   Enter a title, WITHOUT quotation marks.  A maximum of 40 characters  #
C   are allowed.  The default is no title.                               #
C#####
C   TITLE = ' '
C   TITLE = 'CaT'
C   call dtdprx(tout8z,nsave,iset1,iset2,isinc)
C   do 78761 is8z=iset1,iset2,isinc
C   call dtdplo(plout8z,p2out8z,p3out8z,uout8z(0,0,ivar8z,is8z),np1,np
C   &2,0,3,ix8z,jy8z,0,title,vlon,vlat,umin,umax,tout8z(is8z))
78761 continue
C   *****SURFACE PLOTS
C#####
C   Enter a value for IVAR, to select the variable to be plotted or    #
C   printed:                                                            #
C       IVAR = 1 means Ca  (possibly as modified by UPRINT,..)        #
C           2      Cax                                                #
C           3      Cay                                                #
C           4      CaT                                                #
C           5      CaTx                                               #
C           6      CaTy                                               #
C           7      CaC                                                #
C           8      CaCx                                               #
C           9      CaCy                                               #
C          10      CaF                                                #
C          11      CaFx                                               #
C          12      CaFy                                               #
C           .      .                                                  #
C           .      .                                                  #
C#####
C   IVAR =          7
C#####
C   If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC. #
C   #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++
C   + The tabular output or plots will be made at times:                +#+
C   +   T(K) = T0 + K*(TF-T0)/NSAVE                                     +#+
C   + for   K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2          +#+
C   + Enter values for ISET1, ISET2 and ISINC.                          +#+
C   +                                                                     +#+
C   + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular +#+
C   + output or plots will be made at all time values for which the    +#+
C   + solution has been saved.                                          +#+
C   ++++++ END OF "FINE PRINT" ++++++
C#####
C   ISET1 = 0
C   ISET2 = NSAVE
C   ISINC = 1
C#####
C   Enter the view latitude, VLAT, and the view longitude, VLON, desired #
C   for this plot, in degrees.  VLAT and VLON must be between 10 and 80 #
C   degrees; each defaults to 45 degrees.  VLAT and VLON are usually   #
C   defaulted.                                                           #
C#####
C   VLON = 45.0
C   VLAT = 45.0
C
C   ivar8z = ivar + (ivar-1)/3
C   alow = amin8z(ivar8z)
C   ahigh = amax8z(ivar8z)
C#####
C   Specify the range (UMIN,UMAX) for the dependent variable axis.  UMIN #
C   and UMAX are often defaulted.                                       #

```

```

C                                                                 #
C ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#
C + By default, each plot will be scaled to just fit in the plot area. +#
C + For a common scaling, you may want to set UMIN=ALOW, UMAX=AHIGH. +#
C + ALOW and AHIGH are the minimum and maximum values over all output +#
C + points and over all saved time steps or iterations. +#
C ++++++ END OF "FINE PRINT" ++++++#
C#####
C      UMIN = 0.0
C      UMAX = 0.0
C      UMIN =
C & allow
C      UMAX =
C & ahigh
C#####
C      Enter a title, WITHOUT quotation marks. A maximum of 40 characters #
C      are allowed. The default is no title. #
C#####
C      TITLE = ' '
C      TITLE = 'CaC '
C      call dtdprx(tout8z,nsave,iset1,iset2,isinc)
C      do 78762 is8z=iset1,iset2,isinc
C      call dtdplo(plout8z,p2out8z,p3out8z,uout8z(0,0,ivar8z,is8z),np1,np
C      &2,0,3,ix8z,jy8z,0,title,vlon,vlat,umin,umax,tout8z(is8z))
78762 continue
C      *****SURFACE PLOTS
C#####
C      Enter a value for IVAR, to select the variable to be plotted or #
C      printed: #
C      IVAR = 1 means Ca (possibly as modified by UPRINT,..) #
C      2      Cax #
C      3      Cay #
C      4      CaT #
C      5      CaTx #
C      6      CaTy #
C      7      CaC #
C      8      CaCx #
C      9      CaCy #
C      10     CaF #
C      11     CaFx #
C      12     CaFy #
C      .      . #
C      .      . #
C#####
C      IVAR = 10
C#####
C      If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC. #
C      #
C ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#
C + The tabular output or plots will be made at times: +#
C + T(K) = T0 + K*(TF-T0)/NSAVE +#
C + for K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2 +#
C + Enter values for ISET1, ISET2 and ISINC. +#
C + + #
C + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular +#
C + output or plots will be made at all time values for which the +#
C + solution has been saved. +#
C ++++++ END OF "FINE PRINT" ++++++#
C#####
C      ISET1 = 0
C      ISET2 = NSAVE
C      ISINC = 1
C#####
C      Enter the view latitude, VLAT, and the view longitude, VLON, desired #

```

```

C      for this plot, in degrees.  VLAT and VLON must be between 10 and 80      #
C      degrees; each defaults to 45 degrees.  VLAT and VLON are usually      #
C      defaulted.                                                                #
C#####
      VLON = 45.0
      VLAT = 45.0
C
      ivar8z = ivar + (ivar-1)/3
      alow = amin8z(ivar8z)
      ahigh = amax8z(ivar8z)
C#####
C      Specify the range (UMIN,UMAX) for the dependent variable axis.  UMIN    #
C      and UMAX are often defaulted.                                           #
C#####
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++                #
C      + By default, each plot will be scaled to just fit in the plot area.  + #
C      + For a common scaling, you may want to set UMIN=ALOW, UMAX=AHIGH.      + #
C      + ALOW and AHIGH are the minimum and maximum values over all output    + #
C      + points and over all saved time steps or iterations.                  + #
C      ++++++ END OF "FINE PRINT" ++++++                                       #
C#####
      UMIN = 0.0
      UMAX = 0.0
      UMIN =
& alow
      UMAX =
& ahigh
C#####
C      Enter a title, WITHOUT quotation marks.  A maximum of 40 characters    #
C      are allowed.  The default is no title.                                  #
C#####
      TITLE = ' '
      TITLE = 'CaF'
      call dtdprx(tout8z,nsave,iset1,iset2,isinc)
      do 78763 is8z=iset1,iset2,isinc
      call dtdplo(plout8z,p2out8z,p3out8z,uout8z(0,0,ivar8z,is8z),np1,np
&2,0,3,ix8z,jy8z,0,title,vlon,vlat,umin,umax,tout8z(is8z))
78763 continue
C      *****VECTOR PLOTS
C#####
C      Enter values for IVAR1, IVAR2 to select the components Vr1 and Vr2      #
C      of the vector to be plotted.                                           #
C      IVAR1,IVAR2 = 1 means Ca (possibly as modified by UPRINT,...)          #
C          2          Cax                                                       #
C          3          Cay                                                       #
C          4          CaT                                                       #
C          5          CaTx                                                       #
C          6          CaTy                                                       #
C          7          CaC                                                       #
C          8          CaCx                                                       #
C          9          CaCy                                                       #
C          10         CaF                                                       #
C          11         CaFx                                                       #
C          12         CaFy                                                       #
C          .          .                                                         #
C          .          .                                                         #
C      Vr1 and Vr2 are assumed to be the components of the vector in          #
C      Cartesian coordinates.                                                  #
C#####
      IVAR1 =      2
      IVAR2 =      3
C#####
C      If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC.  #
C#####

```

```

C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#
C      + The tabular output or plots will be made at times:      +#
C      +      T(K) = T0 + K*(TF-T0)/NSAVE                        +#
C      + for      K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2  +#
C      + Enter values for ISET1, ISET2 and ISINC.                +#
C      +                                                         +#
C      + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular  +#
C      + output or plots will be made at all time values for which the  +#
C      + solution has been saved.                                +#
C      ++++++ END OF "FINE PRINT" ++++++#
C#####
C      ISET1 = 0
C      ISET2 = NSAVE
C      ISINC = 1
C#####
C      If you don't want to read the FINE PRINT, enter 'no'.      #
C      #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#
C      + Do you want to scale the axes on the plot so that the region is  +#
C      + undistorted? Otherwise the axes will be scaled so that the figure  +#
C      + approximately fills the plot space.                      +#
C      ++++++ END OF "FINE PRINT" ++++++#
C#####
C      NODIST = .FALSE.
C
C      ivr18z = ivar1 + (ivar1-1)/3
C      ivr28z = ivar2 + (ivar2-1)/3
C      almag = max(abs(amin8z(ivr18z)),abs(amax8z(ivr18z)))
C      a2mag = max(abs(amin8z(ivr28z)),abs(amax8z(ivr28z)))
C#####
C      For the purpose of scaling the arrows, the ranges of the two components #
C      of the vector are assumed to be (-VR1MAG,VR1MAG) and (-VR2MAG,VR2MAG). #
C      Enter values for VR1MAG and VR2MAG. VR1MAG and VR2MAG are often #
C      defaulted. #
C      #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#
C      + By default, VR1MAG and VR2MAG are the maxima of the absolute values  +#
C      + of the first and second components. For a common scaling, you may  +#
C      + want to set VR1MAG=A1MAG, VR2MAG=A2MAG. A1MAG, A2MAG are the  +#
C      + maxima of the absolute values over all output points and over all  +#
C      + saved time steps or iterations.                            +#
C      ++++++ END OF "FINE PRINT" ++++++#
C#####
C      VR1MAG = 0.0
C      VR2MAG = 0.0
C#####
C      Enter a title, WITHOUT quotation marks. A maximum of 40 characters #
C      are allowed. The default is no title. #
C#####
C      TITLE = ' '
C      TITLE = 'gradient of Ca '
C      call dtdprx(tout8z,nsave,iset1,iset2,isinc)
C      do 78764 is8z=iset1,iset2,isinc
C      call dtdplq(uout8z(0,0,ivr18z,is8z),uout8z(0,0,ivr28z,is8z),uout8z
C      &(0,0,4,is8z),np1,np2,0,pla,p1b,p2a,p2b,zr8z,zr8z,3,ix8z,jy8z,0,tit
C      &le,vr1mag,vr2mag,zr8z,zr8z,nodist,tout8z(is8z),zr8z,zr8z,zr8z,zr8z
C      &,2,ical8z)
78764 continue
C      *****VECTOR PLOTS
C#####
C      Enter values for IVAR1, IVAR2 to select the components Vr1 and Vr2 #
C      of the vector to be plotted. #
C      IVAR1,IVAR2 = 1 means Ca (possibly as modified by UPRINT,...) #
C      2          Cax #

```

```

C          3          Cay          #
C          4          CaT          #
C          5          CaTx         #
C          6          CaTy         #
C          7          CaC          #
C          8          CaCx         #
C          9          CaCy         #
C         10          CaF          #
C         11          CaFx         #
C         12          CaFy         #
C          .          .           #
C          .          .           #
C      Vr1 and Vr2 are assumed to be the components of the vector in #
C      Cartesian coordinates. #
C#####
C      IVAR1 =          5          #
C      IVAR2 =          6          #
C#####
C      If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC. #
C      #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C      + The tabular output or plots will be made at times: + #
C      +      T(K) = T0 + K*(TF-T0)/NSAVE + #
C      + for      K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2 + #
C      + Enter values for ISET1, ISET2 and ISINC. + #
C      + + #
C      + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular + #
C      + output or plots will be made at all time values for which the + #
C      + solution has been saved. + #
C      ++++++ END OF "FINE PRINT" ++++++ #
C#####
C      ISET1 = 0 #
C      ISET2 = NSAVE #
C      ISINC = 1 #
C#####
C      If you don't want to read the FINE PRINT, enter 'no'. #
C      #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C      + Do you want to scale the axes on the plot so that the region is + #
C      + undistorted? Otherwise the axes will be scaled so that the figure + #
C      + approximately fills the plot space. + #
C      ++++++ END OF "FINE PRINT" ++++++ #
C#####
C      NODIST = .FALSE. #
C #
C      ivr18z = ivar1 + (ivar1-1)/3 #
C      ivr28z = ivar2 + (ivar2-1)/3 #
C      almag = max(abs(amin8z(ivr18z)),abs(amax8z(ivr18z))) #
C      a2mag = max(abs(amin8z(ivr28z)),abs(amax8z(ivr28z))) #
C#####
C      For the purpose of scaling the arrows, the ranges of the two components #
C      of the vector are assumed to be (-VR1MAG,VR1MAG) and (-VR2MAG,VR2MAG). #
C      Enter values for VR1MAG and VR2MAG. VR1MAG and VR2MAG are often #
C      defaulted. #
C      #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C      + By default, VR1MAG and VR2MAG are the maxima of the absolute values + #
C      + of the first and second components. For a common scaling, you may + #
C      + want to set VR1MAG=A1MAG, VR2MAG=A2MAG. A1MAG, A2MAG are the + #
C      + maxima of the absolute values over all output points and over all + #
C      + saved time steps or iterations. + #
C      ++++++ END OF "FINE PRINT" ++++++ #
C#####
C      VR1MAG = 0.0 #

```

```

VR2MAG = 0.0
C#####
C   Enter a title, WITHOUT quotation marks.  A maximum of 40 characters  #
C   are allowed.  The default is no title.                                #
C#####
C   TITLE = ' '
C   TITLE = 'gradient of CaT'
C   call dtdprx(tout8z,nsave,iset1,iset2,isinc)
C   do 78765 is8z=iset1,iset2,isinc
C   call dtdplq(uout8z(0,0,ivr18z,is8z),uout8z(0,0,ivr28z,is8z),uout8z
&(0,0,4,is8z),np1,np2,0,pla,p1b,p2a,p2b,zr8z,zr8z,3,ix8z,jy8z,0,tit
&le,vrlmag,vr2mag,zr8z,zr8z,nodist,tout8z(is8z),zr8z,zr8z,zr8z,zr8z
&,2,ical8z)
78765 continue
C   *****VECTOR PLOTS
C#####
C   Enter values for IVAR1, IVAR2 to select the components Vr1 and Vr2  #
C   of the vector to be plotted.                                         #
C   IVAR1,IVAR2 = 1 means Ca (possibly as modified by UPRINT,...)      #
C   2          Cax                                                         #
C   3          Cay                                                         #
C   4          CaT                                                         #
C   5          CaTx                                                        #
C   6          CaTy                                                        #
C   7          CaC                                                         #
C   8          CaCx                                                        #
C   9          CaCy                                                        #
C   10         CaF                                                         #
C   11         CaFx                                                        #
C   12         CaFy                                                        #
C   .          .                                                           #
C   .          .                                                           #
C   Vr1 and Vr2 are assumed to be the components of the vector in      #
C   Cartesian coordinates.                                               #
C#####
C   IVAR1 =      8
C   IVAR2 =      9
C#####
C   If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC. #
C   #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++
C   + The tabular output or plots will be made at times:                +
C   + T(K) = T0 + K*(TF-T0)/NSAVE                                       +
C   + for K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2              +
C   + Enter values for ISET1, ISET2 and ISINC.                            +
C   +                                                                       +
C   + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular +
C   + output or plots will be made at all time values for which the     +
C   + solution has been saved.                                           +
C   ++++++ END OF "FINE PRINT" ++++++
C#####
C   ISET1 = 0
C   ISET2 = NSAVE
C   ISINC = 1
C#####
C   If you don't want to read the FINE PRINT, enter 'no'.              #
C   #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++
C   + Do you want to scale the axes on the plot so that the region is   +
C   + undistorted?  Otherwise the axes will be scaled so that the figure +
C   + approximately fills the plot space.                                +
C   ++++++ END OF "FINE PRINT" ++++++
C#####
C   NODIST = .FALSE.

```

```

C
  ivr18z = ivar1 + (ivar1-1)/3
  ivr28z = ivar2 + (ivar2-1)/3
  almag = max(abs(amin8z(ivr18z)),abs(amax8z(ivr18z)))
  a2mag = max(abs(amin8z(ivr28z)),abs(amax8z(ivr28z)))
C#####
C   For the purpose of scaling the arrows, the ranges of the two components #
C   of the vector are assumed to be (-VR1MAG,VR1MAG) and (-VR2MAG,VR2MAG). #
C   Enter values for VR1MAG and VR2MAG. VR1MAG and VR2MAG are often #
C   defaulted. #
C #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C   + By default, VR1MAG and VR2MAG are the maxima of the absolute values + #
C   + of the first and second components. For a common scaling, you may + #
C   + want to set VR1MAG=A1MAG, VR2MAG=A2MAG. A1MAG, A2MAG are the + #
C   + maxima of the absolute values over all output points and over all + #
C   + saved time steps or iterations. + #
C   ++++++ END OF "FINE PRINT" ++++++ #
C#####
  VR1MAG = 0.0
  VR2MAG = 0.0
C#####
C   Enter a title, WITHOUT quotation marks. A maximum of 40 characters #
C   are allowed. The default is no title. #
C#####
  TITLE = ' '
  TITLE = 'gradient of CaC '
  call dtdprx(tout8z,nsave,iset1,iset2,isinc)
  do 78766 is8z=iset1,iset2,isinc
    call dtdplq(uout8z(0,0,ivr18z,is8z),uout8z(0,0,ivr28z,is8z),uout8z
&(0,0,4,is8z),np1,np2,0,p1a,p1b,p2a,p2b,zr8z,zr8z,3,ix8z,jy8z,0,tit
&le,vr1mag,vr2mag,zr8z,zr8z,nodist,tout8z(is8z),zr8z,zr8z,zr8z,zr8z
&,2,ical8z)
78766 continue
C   *****VECTOR PLOTS
C#####
C   Enter values for IVAR1, IVAR2 to select the components Vr1 and Vr2 #
C   of the vector to be plotted. #
C   IVAR1,IVAR2 = 1 means Ca (possibly as modified by UPRINT,...) #
C   2 CaX #
C   3 CaY #
C   4 CaT #
C   5 CaTx #
C   6 CaTy #
C   7 CaC #
C   8 CaCx #
C   9 CaCy #
C   10 CaF #
C   11 CaFx #
C   12 CaFy #
C   . #
C   . #
C   Vr1 and Vr2 are assumed to be the components of the vector in #
C   Cartesian coordinates. #
C#####
  IVAR1 = 11
  IVAR2 = 12
C#####
C   If you don't want to read the FINE PRINT, default ISET1,ISET2,ISINC. #
C #
C   ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C   + The tabular output or plots will be made at times: + #
C   + T(K) = T0 + K*(TF-T0)/NSAVE + #
C   + for K = ISET1, ISET1+ISINC, ISET1+2*ISINC,..., ISET2 + #

```

```

C      + Enter values for ISET1, ISET2 and ISINC.                + #
C      +                                                         + #
C      + The default is ISET1=0, ISET2=NSAVE, ISINC=1, that is, the tabular + #
C      + output or plots will be made at all time values for which the + #
C      + solution has been saved.                                  + #
C      ++++++ END OF "FINE PRINT" ++++++
C#####
      ISET1 = 0
      ISET2 = NSAVE
      ISINC = 1
C#####
C      If you don't want to read the FINE PRINT, enter 'no'.    #
C      #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C      + Do you want to scale the axes on the plot so that the region is + #
C      + undistorted? Otherwise the axes will be scaled so that the figure + #
C      + approximately fills the plot space.                       + #
C      ++++++ END OF "FINE PRINT" ++++++
C#####
      NODIST = .FALSE.
C
      ivr18z = ivar1 + (ivar1-1)/3
      ivr28z = ivar2 + (ivar2-1)/3
      almag = max(abs(amin8z(ivr18z)),abs(amax8z(ivr18z)))
      a2mag = max(abs(amin8z(ivr28z)),abs(amax8z(ivr28z)))
C#####
C      For the purpose of scaling the arrows, the ranges of the two components #
C      of the vector are assumed to be (-VR1MAG,VR1MAG) and (-VR2MAG,VR2MAG). #
C      Enter values for VR1MAG and VR2MAG. VR1MAG and VR2MAG are often #
C      defaulted.                                               #
C      #
C      ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++ #
C      + By default, VR1MAG and VR2MAG are the maxima of the absolute values + #
C      + of the first and second components. For a common scaling, you may + #
C      + want to set VR1MAG=A1MAG, VR2MAG=A2MAG. A1MAG, A2MAG are the + #
C      + maxima of the absolute values over all output points and over all + #
C      + saved time steps or iterations.                         + #
C      ++++++ END OF "FINE PRINT" ++++++
C#####
      VR1MAG = 0.0
      VR2MAG = 0.0
C#####
C      Enter a title, WITHOUT quotation marks. A maximum of 40 characters #
C      are allowed. The default is no title.                    #
C#####
      TITLE = ' '
      TITLE = 'gradient of CaF '
      call dtdprx(tout8z,nsave,iset1,iset2,isinc)
      do 78767 is8z=iset1,iset2,isinc
      call dtdplq(uout8z(0,0,ivr18z,is8z),uout8z(0,0,ivr28z,is8z),uout8z
&(0,0,4,is8z),np1,np2,0,p1a,p1b,p2a,p2b,zr8z,zr8z,3,ix8z,jy8z,0,tit
&le,vr1mag,vr2mag,zr8z,zr8z,nodist,tout8z(is8z),zr8z,zr8z,zr8z,zr8z
&,2,ical8z)
78767 continue
78755 continue
      call endgks
      stop
      end

      subroutine tran8z(itrans,p1,p2,p38z)
      implicit double precision (a-h,o-z)
      common /dtdp41/x,y,z8z,x1,x2,x3,y1,y2,y3,z1,z2,z3,x11,x21,x31,x12,
&x22,x32,x13,x23,x33,y11,y21,y31,y12,y22,y32,y13,y23,y33,z11,z21,z3

```



```

&l,z12,z22,z32,z13,z23,z33
common/parm8z/pi,DCA,Umax,EC50 ,Hill,CArest,RC,Aca
&,OD2,Slope ,Slope2,Width,TN,Flu,Cal,ktn_p,ktn_n,kcal_p
&,kflu_n,DCal,Dflu ,DU ,OTB ,kcal_n, kflu_p
C#####
C You can solve problems in your region only if you can describe it by #
C X = X(P1,P2) #
C Y = Y(P1,P2) #
C with constant limits on the parameters P1,P2. If your region is #
C rectangular, enter ITRANS=0 and the trivial parameterization #
C X = P1 #
C Y = P2 #
C will be used. Otherwise, you need to read the FINE PRINT below. #
C #
C ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#
C + If P1,P2 represent polar or other non-Cartesian coordinates, you can +#
C + reference the Cartesian coordinates X,Y and derivatives of your +#
C + unknowns with respect to these coordinates, when you define your +#
C + PDE coefficients, boundary conditions, and volume and boundary +#
C + integrals, if you enter ITRANS .NE. 0. Enter: +#
C + ITRANS = 1, if P1,P2 are polar coordinates, that is, if +#
C + P1=R, P2=Theta, where X = R*cos(Theta) +#
C + Y = R*sin(Theta) +#
C + ITRANS = -1, same as ITRANS=1, but P1=Theta, P2=R +#
C + ITRANS = 3, to define your own coordinate transformation. In +#
C + this case, you will be prompted to define X,Y and +#
C + their first and second derivatives in terms of P1,P2. +#
C + Because of symmetry, you will not be prompted for all +#
C + of the second derivatives. If you make a mistake in +#
C + computing any of these derivatives, PDE2D will usually +#
C + be able to issue a warning message. (X1 = dX/dP1, etc) +#
C + ITRANS = -3, same as ITRANS=3, but you will only be prompted to +#
C + define X,Y; their first and second derivatives will +#
C + be approximated using finite differences. +#
C + When ITRANS = -3 or 3, the first derivatives of X,Y must all be +#
C + continuous. +#
C ++++++ END OF "FINE PRINT" ++++++#
C#####
ITRANS = 0
return
end

subroutine pdes8z(yd8z,i8z,j8z,kint8z,p1,p2,p38z,t,uu8z)
implicit double precision (a-h,o-z)

INTEGER :: gg,jj
REAL,DIMENSION(0:2000,0:1000)::td1,tb1,tb2,td2,tb3,td3,tb4,td4

REAL:: mv=0

parameter (neqnm= 99)
C un8z(1,I),un8z(2,I),... hold the (rarely used) values
C of UI,UI1,... from the previous iteration or time step
common /dtdp5x/un8z(10,neqnm)
common /dtdp18/norm1,norm2,n38z
double precision norm1,norm2,n38z,normx,normy,nz8z
dimension uu8z(10,neqnm)
common/parm8z/pi,DCA,Umax,EC50 ,Hill,CArest,RC,Aca
&,OD2,Slope ,Slope2,Width,TN,Flu,Cal,ktn_p,ktn_n,kcal_p
&,kflu_n,DCal,Dflu ,DU ,OTB ,kcal_n, kflu_p
zr8z = 0.0
Ca = uu8z(1, 1)
Cal = uu8z(2, 1)

```





```

C                                                                 #
C   The parameters P1,P2 and derivatives with respect to these may also #
C   be referenced (Ca1 = dCa/dP1, etc):                               #
C       Ca1,Ca2,Ca11,Ca22,Ca12                                       #
C       CaT1,CaT2,CaT11,CaT22,CaT12                                  #
C       CaC1,CaC2,CaC11,CaC22,CaC12                                  #
C       CaF1,CaF2,CaF11,CaF22,CaF12                                  #
C                                                                 #
C#####
C@@@ Partial Differential Equations
      o=1
      z=1
C-----Rate constant for release generator of region #2 -----
      Rk=3
C--Rate constant for luminal Ca2+ depletion effect on Ca2+ release of region #2
      Kc=3.2
C--Rate constant for luminal Ca2+ depletion effect on Ca2+ release of region #1
C--and #3 -----
      Kb=5
C-----variable time offset for initial trigger-----
      DU1=0
C-----Time base for initial trigger-----
      OTB1=100
C-----Slope1 for region #2 release generator-----
      Slope1=80
C-----Pulse modulator for region #2 release generator-----
      Pulse1=36
      UD=0.06
C-----Slope2 for region #2 release generator-----
      Slope3=UD*Slope1
C-----Deactivating parameter for region #2 release generator-----

C*****

      iF (x.lt.1.or.x.gt.28) THEN
C----RR1=Initial trigger , RR2= Release from region #1 and #3 , RR3= Release of
C----region #2-----
      RR1=0
      RR2=0
      RR3=0
      ELSE

C   RU= Uptake and RL=leak from the SR.
      RU=0
      RL=0
C----- Release generator location-----
      gg=nint((x*20))
      jj=nint((y*20))

c=====SERCA PUMP activation =====

      v2=gg-v3

      if(v2.eq.35.or.v2.eq.0.or.v2.eq.36.or.gg.eq.28) then
        v3=gg
        RU =(Umax*Ca**Hill)/(EC50**Hill + Ca**Hill)
        RL =(Umax*CArest**Hill)/(EC50**Hill + CArest**Hill)
      endif

c=== Time to reach an equilibrium before any release to set resting [Ca]===
C----- Tequ= Time of equilibrium-----
      Tequ=0.015

```

```

if (t.le.Tequ) then

    RR1=0
    RR2=0
    RR3=0
    else

C=====
    IF (t.lt.0.001) then
C    time initiation delay . b stores time not releasing.
        b = t
        RR1 = 0.0
        nn=0

C=====
    ELSE
        RR1=0
        RR3=0
C-----tt= time counter for initial release-----
        tt = t-Tequ
C----- Ca release expression terms -----

        DN1 = 1.0 + exp(Slope1*(DU1-OTB1*tt))
        DN2 = 1.0 + exp(OD3 + Slope3*(DU1-OTB1*tt))

c=====Release locations of RYR=====

        v4=gg-v5

        if (gg.eq.43.or.v4.eq.36.or.v4.eq.0.or.v4.eq.35.
& and.gg.lt.527) then

            v5=gg

c=====Initial release at region #1=====

            if (y.ge.0.9.and.y.le.2) then

C----- Ca release expression -----

                RR1=1200*exp(-Kc*tt)*(CArest/Ca)*(exp(-Rk*tt)/DN1-1/DN2)

                endif

            if(y.gt.0.9.and.y.lt.3) then

C----- Threshold of activation for release generator at region #2-----

                if (Ca.lt.0.107) then

                    tb1(gg,jj)=t
                    RR3=0
                else

C-----td1= Release location specific time counter at region #2-----

                    td1(gg,jj)=t-tb1(gg,jj)-Tequ
                    DN3 = 1.0 + exp(Slope1*(-OTB*td1(gg,jj)))
                    DN4 = 1.0 + exp(OD3 + Slope3*(-OTB*td1(gg,jj)))

```

```

if (exp(-RC*td1(gg,jj)).gt.(1/DN3 - 1/DN4)) then
    RR3=0

else

    kt1 = td1(gg,jj)
C----- Ca release expression -----
    RR3=1200*exp(-Kc*tt)*(CArest/Ca)*(exp(-Rk*kt1)/DN3-1/DN4)

    endif
    endif
    endif

c-----Region #1 release-----
    IF(y.gt.0.9.and.y.le.2.3) then

        if (Ca.lt.0.14) then

            tb2(gg,jj)=t
            RR2=0.0

        else
C-----td2= Release location specific time counter at region #1-----
            td2(gg,jj)=t-tb2(gg,jj)-Tequ
            D1 = 1.0 + exp(Slope*(-OTB*td2(gg,jj)))
            D2 = 1.0 + exp(OD2 + Slope2*(-OTB*td2(gg,jj)))

            if (exp(-RC*td2(gg,jj)).gt.(1/D1 - 1/D2)) then

                RR2=0

            else
                kt2 = td2(gg,jj)
C----- Ca release expression -----
                RR2=exp(-Kb*tt)*1200*(CArest/Ca)*(exp(-RC*kt2)/D1-1/D2)

                endif

            endif
        ENDIF

c=====Region #3 release =====

        IF(y.gt.3) then
            RR3=0

c ----- threshold of activation for region #3-----

            if (Ca.lt.0.14) then

                tb4(gg,jj)=t
                RR2=0.0

```

```

        yp=0
    else
C-----td4= Release location specific time counter at region #3-----
        td4(gg,jj)=t-tb4(gg,jj)-Tequ

        D1 = 1.0 + exp(Slope*(-OTB*td4(gg,jj)))
        D2 = 1.0 + exp(OD2 + Slope2*(-OTB*td4(gg,jj)))

        if (exp(-RC*td4(gg,jj)).gt.(1/D1 - 1/D2)) then

            RR2=0

        else

            kt4 = td4(gg,jj)
C----- Ca release expression -----
            RR2=exp(-Kb*tt)*1200*(CArest/Ca)*(exp(-RC*kt4)/D1-1/D2)

        endif

    endif

endif

ENDIF

C=====

C*****
endif

endif

    if(RR1.lt.0.0) then
        RR1=0.0
    endif

    if(RR2.lt.0.0) then
        RR2=0.0
    endif

endif
ENDIF

C=====

        if (j8z.eq.0) then
            yd8z = 0.0
C-----> INPUT FROM GUI <-----
C                                     C(1,1) DEFINED
C         if (i8z.eq. -101) yd8z =
            & 1                                     C(1,2) DEFINED
C         if (i8z.eq. -102) yd8z =
            & 0                                     C(1,3) DEFINED
C         if (i8z.eq. -103) yd8z =
            & 0

```

```

C
    if (i8z.eq. -104) yd8z =
& 0
C-----> INPUT FROM GUI <-----
C
    F1 DEFINED
C-----System of PDEs expression -----

    if (i8z.eq. 1) yd8z =
& DCA*(Caxx+Cayy)+RL + RR1+RR2+RR3-RU-ktn_p*(TN-CaT)*Ca
& +ktn_n*CaT -kcal_p*(Cal-CaC)*Ca+kcal_n*CaC-kflu_p*(Flu-CaF)
& *Ca+kflu_n*CaF

C-----> INPUT FROM GUI <-----
C
    C (2,1) DEFINED
    if (i8z.eq. -201) yd8z =
& 0
C
    C (2,2) DEFINED
    if (i8z.eq. -202) yd8z =
& 1
C
    C (2,3) DEFINED
    if (i8z.eq. -203) yd8z =
& 0
C
    C (2,4) DEFINED
    if (i8z.eq. -204) yd8z =
& 0
C-----> INPUT FROM GUI <-----
C
    F2 DEFINED
C-----For Troponin C-----
    if (i8z.eq. 2) yd8z =
& ktn_p*(TN-CaT)*Ca-ktn_n*CaT
C-----> INPUT FROM GUI <-----
C
    C (3,1) DEFINED
    if (i8z.eq. -301) yd8z =
& 0
C
    C (3,2) DEFINED
    if (i8z.eq. -302) yd8z =
& 0
C
    C (3,3) DEFINED
    if (i8z.eq. -303) yd8z =
& 1
C
    C (3,4) DEFINED
    if (i8z.eq. -304) yd8z =
& 0
C-----> INPUT FROM GUI <-----
C
    F3 DEFINED
C-----For Calmodulin-----
    if (i8z.eq. 3) yd8z =
& DCal*(CaCxx+CaCyy)+kcal_p*(Cal-CaC)*Ca-kcal_n*CaC
C-----> INPUT FROM GUI <-----
C
    C (4,1) DEFINED
    if (i8z.eq. -401) yd8z =
& 0
C
    C (4,2) DEFINED
    if (i8z.eq. -402) yd8z =
& 0
C
    C (4,3) DEFINED
    if (i8z.eq. -403) yd8z =
& 0
C
    C (4,4) DEFINED
    if (i8z.eq. -404) yd8z =
& 1
C-----> INPUT FROM GUI <-----
C
    F4 DEFINED

```



```

C-----For Fluo4-----
      if (i8z.eq. 4) yd8z =
& Dflu*(CaFxx+CaFyy)+kflu_p*(Flu-CaF)*Ca-kflu_n*CaF
          else
          endif
      endif

      return
      end

      function u8z(i8z,p1,p2,p38z,t0)
      implicit double precision (a-h,o-z)
      common/parm8z/pi,DCA,Umax,EC50 ,Hill,CArest,RC,Aca
& ,OD2,Slope ,Slope2,Width,TN,Flu,Cal,ktn_p,ktn_n,kcal_p
& ,kflu_n,DCal,Dflu ,DU ,OTB ,kcal_n, kflu_p
      call dtdpcd(p1,p2,p38z)
      call dtdpcb(p1,p2,p38z,z18z,z28z,z38z,x,y,z8z,d18z,d28z,d38z,1)
      u8z = 0.0
C#####
C      Now the initial values must be defined using FORTRAN expressions.      #
C      They may be functions of X and Y (and the parameters P1,P2), and may      #
C      also reference the initial time T0.      #
C#####

C=====Initial Conditions=====

C-----> INPUT FROM GUI <-----
C-----Initial Ca concentration-----
C
      Ca0 DEFINED
      if (i8z.eq. 1) u8z =
& 0.1

C-----> INPUT FROM GUI <-----
C-----Initial Ca-Troponin concentration-----
C
      CaT0 DEFINED
      if (i8z.eq. 2) u8z =
& 6.5271

C-----> INPUT FROM GUI <-----
C-----Initial Ca-Calmodulin concentration-----
C
      CaC0 DEFINED
      if (i8z.eq. 3) u8z =
& 0.9677

C-----> INPUT FROM GUI <-----
C-----Initial Ca-Fluo4 concentration-----
C
      CaF0 DEFINED
      if (i8z.eq. 4) u8z =
& 11.91709845

      return
      end

      subroutine gb8z(gd8z,ifac8z,i8z,j8z,p1,p2,p38z,t,uu8z)
      implicit double precision (a-h,o-z)
      parameter (neqnmx= 99)
      dimension uu8z(10,neqnmx)
C      un8z(1,I),un8z(2,I),... hold the (rarely used) values
C      of UI,UI1,... from the previous iteration or time step
      common /dtdp5x/ un8z(10,neqnmx)
      common /dtdp18/norm1,norm2,n38z
      double precision none,norm1,norm2,n38z,normx,normy,nz8z
      common/parm8z/pi,DCA,Umax,EC50 ,Hill,CArest,RC,Aca
& ,OD2,Slope ,Slope2,Width,TN,Flu,Cal,ktn_p,ktn_n,kcal_p

```

```

&,kflu_n,DCal,Dflu ,DU ,OTB ,kcal_n, kflu_p
none = dtdplx(2)
zr8z = 0.0
Ca = uu8z(1, 1)
Ca1 = uu8z(2, 1)
Ca2 = uu8z(3, 1)
CaT = uu8z(1, 2)
CaT1 = uu8z(2, 2)
CaT2 = uu8z(3, 2)
CaC = uu8z(1, 3)
CaC1 = uu8z(2, 3)
CaC2 = uu8z(3, 3)
CaF = uu8z(1, 4)
CaF1 = uu8z(2, 4)
CaF2 = uu8z(3, 4)
call dtdpcd(p1,p2,p38z)
call dtdpcb(p1,p2,p38z,norm1,norm2,n38z,x,y,z8z,normx,normy,nz8z,3
&)
call dtdpcb(
& p1,p2,p38z,Ca1,Ca2,zr8z,x,y,z8z,Cax,Cay,uz8z,2)
Canorm = Cax*normx + Cay*normy
call dtdpcb(
& p1,p2,p38z,CaT1,CaT2,zr8z,x,y,z8z,CaTx,CaTy,uz8z,2)
CaTnorm = CaTx*normx + CaTy*normy
call dtdpcb(
& p1,p2,p38z,CaC1,CaC2,zr8z,x,y,z8z,CaCx,CaCy,uz8z,2)
CaCnorm = CaCx*normx + CaCy*normy
call dtdpcb(
& p1,p2,p38z,CaF1,CaF2,zr8z,x,y,z8z,CaFx,CaFy,uz8z,2)
CaFnorm = CaFx*normx + CaFy*normy
if (j8z.eq.0) gd8z = 0.0
C#####
C Enter FORTRAN expressions to define the boundary condition functions, #
C which may be functions of #
C # #
C X,Y,Ca,Cax,Cay, #
C CaT,CaTx,CaTy, #
C CaC,CaCx,CaCy, #
C CaF,CaFx,CaFy and (if applicable) T #
C . . . #
C # #
C Recall that the boundary conditions have the form #
C # #
C G1 = 0 #
C G2 = 0 #
C G3 = 0 #
C G4 = 0 #
C . . #
C Enter NONE to indicate "no" boundary condition. #
C # #
C The parameters P1,P2 and derivatives with respect to these may also #
C be referenced (Ca1 = dCa/dP1, etc): #
C Ca1,Ca2 #
C CaT1,CaT2 #
C CaC1,CaC2 #
C CaF1,CaF2 #
C . . #
C The components (NORMx,NORMy) of the unit outward normal vector #
C may also be referenced, as well as the normal derivatives Canorm, #
C CaTnorm,CaCnorm,CaFnorm... #
C # #
C ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#
C + If "no" boundary condition is specified, the corresponding PDE is + #
C + enforced at points just inside the boundary (exactly on the + #

```

```

C      + boundary, if EPS8Z is set to 0 in the main program).          +#+
C      ++++++ END OF "FINE PRINT" ++++++                               +#+
C#####
C      if (ifac8z.eq. 1) then
C#####
C      #
C      First define the boundary conditions on the face P1 = P1GRID(1).  #
C#####
C      if (j8z.eq.0) then
C-----> INPUT FROM GUI <-----
C      G1 DEFINED
C      if (i8z.eq. 1) gd8z =
C      & Ca-0.1
C-----> INPUT FROM GUI <-----
C      G2 DEFINED
C      if (i8z.eq. 2) gd8z =
C      & CaT-6.5271
C-----> INPUT FROM GUI <-----
C      G3 DEFINED
C      if (i8z.eq. 3) gd8z =
C      & CaC-0.9677
C-----> INPUT FROM GUI <-----
C      G4 DEFINED
C      if (i8z.eq. 4) gd8z =
C      & CaF-11.91709845
C      else
C      endif
C      endif
C      if (ifac8z.eq. 2) then
C#####
C      #
C      Now define the boundary conditions on the face P1 = P1GRID(NP1GRID). #
C#####
C      if (j8z.eq.0) then
C-----> INPUT FROM GUI <-----
C      G1 DEFINED
C      if (i8z.eq. 1) gd8z =
C      & Ca-0.1
C-----> INPUT FROM GUI <-----
C      G2 DEFINED
C      if (i8z.eq. 2) gd8z =
C      & CaT-6.5271
C-----> INPUT FROM GUI <-----
C      G3 DEFINED
C      if (i8z.eq. 3) gd8z =
C      & CaC-0.9677
C-----> INPUT FROM GUI <-----
C      G4 DEFINED
C      if (i8z.eq. 4) gd8z =
C      & CaF-11.91709845
C      else
C      endif
C      endif
C      if (ifac8z.eq. 3) then
C#####
C      #
C      Now define the boundary conditions on the face P2 = P2GRID(1).  #
C#####
C      if (j8z.eq.0) then
C-----> INPUT FROM GUI <-----
C      G1 DEFINED
C      if (i8z.eq. 1) gd8z =
C      & Ca-0.1

```

```

C-----> INPUT FROM GUI <-----
C                                     G2 DEFINED
      if (i8z.eq.    2) gd8z =
      & CaT-6.5271
C-----> INPUT FROM GUI <-----
C                                     G3 DEFINED
      if (i8z.eq.    3) gd8z =
      & CaC-0.9677
C-----> INPUT FROM GUI <-----
C                                     G4 DEFINED
      if (i8z.eq.    4) gd8z =
      & CaF-11.91709845
                                     else
                                     endif
      endif
      if (ifac8z.eq. 4) then
C#####
C                                     #
C      Now define the boundary conditions on the face P2 = P2GRID(NP2GRID).  #
C#####
      if (j8z.eq.0) then
C-----> INPUT FROM GUI <-----
C                                     G1 DEFINED
      if (i8z.eq.    1) gd8z =
      & Ca-0.1
C-----> INPUT FROM GUI <-----
C                                     G2 DEFINED
      if (i8z.eq.    2) gd8z =
      & CaT-6.5271
C-----> INPUT FROM GUI <-----
C                                     G3 DEFINED
      if (i8z.eq.    3) gd8z =
      & CaC-0.9677
C-----> INPUT FROM GUI <-----
C                                     G4 DEFINED
      if (i8z.eq.    4) gd8z =
      & CaF-11.91709845
                                     else
                                     endif
      endif
      return
      end

subroutine pmod8z(p1,p2,p38z,t,uu8z,uprint,uxprnt,uyprnt,uzpr8z)
implicit double precision (a-h,o-z)
dimension uu8z(10,*),uprint(*),uxprnt(*),uyprnt(*),uzpr8z(*)
common/dtdp14/sint(20),bint(20),slim8z(20),blim8z(20)
common/parm8z/pi,DCA,Umax,EC50 ,Hill,CArest,RC,Aca
&,OD2,Slope ,Slope2,Width,TN,Flu,Cal,ktn_p,ktn_n,kcal_p
&,kflu_n,DCal,Dflu ,DU ,OTB ,kcal_n, kflu_p
zr8z = 0.0
Ca  = uu8z(1, 1)
Ca1 = uu8z(2, 1)
Ca2 = uu8z(3, 1)
Ca11= uu8z(5, 1)
Ca22= uu8z(6, 1)
Ca12= uu8z(8, 1)
Ca21= uu8z(8, 1)
CaT  = uu8z(1, 2)
CaT1 = uu8z(2, 2)
CaT2 = uu8z(3, 2)
CaT11= uu8z(5, 2)
CaT22= uu8z(6, 2)

```

```

CaT12= uu8z(8, 2)
CaT21= uu8z(8, 2)
CaC  = uu8z(1, 3)
CaC1 = uu8z(2, 3)
CaC2 = uu8z(3, 3)
CaC11= uu8z(5, 3)
CaC22= uu8z(6, 3)
CaC12= uu8z(8, 3)
CaC21= uu8z(8, 3)
CaF  = uu8z(1, 4)
CaF1 = uu8z(2, 4)
CaF2 = uu8z(3, 4)
CaF11= uu8z(5, 4)
CaF22= uu8z(6, 4)
CaF12= uu8z(8, 4)
CaF21= uu8z(8, 4)
call dtdpcd(p1,p2,p38z)
call dtdpcc(p1,p2,p38z,
&          Ca1,Ca2,zr8z,Ca11,Ca22,zr8z,Ca12,zr8z,zr8z,
& x,y,z8z,Cax,Cay,uz8z,Caxx,Cayy,uzz8z,Caxy,uxz8z,uyz8z,
& Cayx,uzx8z,zy8z,dvol8z,dare8z)
uxprnt( 1) = Cax
uyprnt( 1) = Cay
call dtdpcc(p1,p2,p38z,
&          CaT1,CaT2,zr8z,CaT11,CaT22,zr8z,CaT12,zr8z,zr8z,
& x,y,z8z,CaTx,CaTy,uz8z,CaTxx,CaTyy,uzz8z,CaTxy,uxz8z,uyz8z,
& CaTyx,uzx8z,zy8z,dvol8z,dare8z)
uxprnt( 2) = CaTx
uyprnt( 2) = CaTy
call dtdpcc(p1,p2,p38z,
&          CaC1,CaC2,zr8z,CaC11,CaC22,zr8z,CaC12,zr8z,zr8z,
& x,y,z8z,CaCx,CaCy,uz8z,CaCxx,CaCyy,uzz8z,CaCxy,uxz8z,uyz8z,
& CaCyx,uzx8z,zy8z,dvol8z,dare8z)
uxprnt( 3) = CaCx
uyprnt( 3) = CaCy
call dtdpcc(p1,p2,p38z,
&          CaF1,CaF2,zr8z,CaF11,CaF22,zr8z,CaF12,zr8z,zr8z,
& x,y,z8z,CaFx,CaFy,uz8z,CaFxx,CaFyy,uzz8z,CaFxy,uxz8z,uyz8z,
& CaFyx,uzx8z,zy8z,dvol8z,dare8z)
uxprnt( 4) = CaFx
uyprnt( 4) = CaFy
C#####
C  If you don't want to read the FINE PRINT, default all of the following #
C  variables.                                                                #
C                                                                                   #
C  ++++++ THE "FINE PRINT" (CAN USUALLY BE IGNORED) ++++++#####
C  + Normally, PDE2D saves the values of Ca,Cax,Cay,CaT,CaTx,CaTy,          +#
C  + CaC,CaCx,CaCy,CaF,CaFx,CaFy...at the output points.  If different      +#
C  + variables are to be saved (for later printing or plotting) the        +#
C  + following functions can be used to re-define the output variables:    +#
C  +   define UPRINT(1) to replace  Ca                                     +#
C  +           UXPRT(1)              Cax                                  +#
C  +           UYPRNT(1)             Cay                                  +#
C  +           UPRINT(2)             CaT                                  +#
C  +           UXPRT(2)              CaTx                                 +#
C  +           UYPRNT(2)             CaTy                                 +#
C  +           UPRINT(3)             CaC                                  +#
C  +           UXPRT(3)              CaCx                                 +#
C  +           UYPRNT(3)             CaCy                                 +#
C  +           UPRINT(4)             CaF                                  +#
C  +           UXPRT(4)              CaFx                                 +#
C  +           UYPRNT(4)             CaFy                                 +#
C  +           .                      .                                  +#
C  +           .                      .                                  +#

```

```

C      + Each function may be a function of                                +##
C      +                                                                    +##
C      +      X, Y, Ca, Cax, Cay, Caxx, Cayy, Caxy                          +##
C      +      CaT, CaTx, CaTy, CaTxx, CaTyy, CaTxy                          +##
C      +      CaC, CaCx, CaCy, CaCxx, CaCyy, CaCxy                          +##
C      +      CaF, CaFx, CaFy, CaFxx, CaFyy, CaFxy and (if applicable) T    +##
C      +      . . . . .                                                    +##
C      +                                                                    +##
C      + Each may also be a function of the integral estimates SINT(1),..., +##
C      + BINT(1),...                                                       +##
C      +                                                                    +##
C      + The parameters P1,P2 and derivatives with respect to these may also +##
C      + be referenced (Ca1 = dCa/dP1, etc):                                +##
C      +      Ca1,Ca2,Ca11,Ca22,Ca12                                         +##
C      +      CaT1,CaT2,CaT11,CaT22,CaT12                                    +##
C      +      CaC1,CaC2,CaC11,CaC22,CaC12                                    +##
C      +      CaF1,CaF2,CaF11,CaF22,CaF12                                    +##
C      +      . . . . .                                                    +##
C      +                                                                    +##
C      + The default for each variable is no change, for example, UPRINT(1) +##
C      + defaults to Ca. Enter FORTRAN expressions for each of the         +##
C      + following functions (or default).                                    +##
C      ++++++ END OF "FINE PRINT" ++++++ +##
C#####
C      DEFINE UPRINT(*),UXPRNT(*),UYPRNT(*) HERE:
      return
      end

      function axis8z(i8z,p1,p2,p38z,ical8z)
      implicit double precision (a-h,o-z)
      call dtdpcd(p1,p2,p38z)
      call dtdpcb(p1,p2,p38z,z18z,z28z,z38z,x,y,z8z,d18z,d28z,d38z,1)
      if (i8z.eq.1) axis8z = x
      if (i8z.eq.2) axis8z = y
      return
      end

C      dummy routines
      subroutine xy8z(i8z,iarc8z,s,x,y,s0,sf)
      implicit double precision (a-h,o-z)
      return
      end
      subroutine dis8z(x,y,ktri,triden,shape)
      implicit double precision (a-h,o-z)
      return
      end
      function fb8z(i8z,iarc8z,ktri,s,x,y,t)
      implicit double precision (a-h,o-z)
      fb8z = 0
      return
      end

      subroutine postpr(tout,nsave,plout,p2out,np1,np2,uout,neqn)
      implicit double precision (a-h,o-z)
      dimension plout(0:np1,0:np2),p2out(0:np1,0:np2),tout(0:nsave)
      dimension uout(0:np1,0:np2,4,neqn,0:nsave)
      common/parm8z/pi,DCA,Umax,EC50 ,Hill,CArest,RC,Aca
      &,OD2,Slope ,Slope2,Width,TN,Flu,Cal,ktn_p,ktn_n,kcal_p
      &,kflu_n,DCal,Dflu ,DU ,OTB ,kcal_n, kflu_p
      common /dtdp27/ itask,npes,icommm
      common /dtdp46/ eps8z,cgtl8z,npmx8z,itYPE,near8z
      data lun,lud/0,47/
      if (itask.gt.0) return

```

```

C      UOUT(I,J,IDER,IEQ,L) = U-sub-IEQ,  if IDER=1
C                                  Ux-sub-IEQ, if IDER=2
C                                  Uy-sub-IEQ, if IDER=3
C      (possibly as modified by UPRINT,..)
C      at the point (P1OUT(I,J) , P2OUT(I,J))
C      at time/iteration TOUT(L).
C      ***** ADD POSTPROCESSING CODE HERE:
C      IN THE EXAMPLE BELOW, MATLAB PLOTFILES pde2d.m,
C      pde2d.rdm CREATED (REMOVE COMMENTS TO ACTIVATE)
if (lun.eq.0) then
    lun = 46
    open (lun,file='pde2d.m')
    open (lud,file='pde2d.rdm')
    write (lun,*) 'fid = fopen(''pde2d.rdm'');'
endif
do 78753 l=0,nsave
    if (tout(l).ne.dtdplx(2)) nsave0 = 1
78753 continue
    write (lud,78754) nsave0
    write (lud,78754) neqn
    write (lud,78754) np1
    write (lud,78754) np2
78754 format (i8)
    do 78756 i=0,np1
    do 78755 j=0,np2
        p1 = plout(i,j)
        p2 = p2out(i,j)
        p38z = 0.0
        call dtdpcd(p1,p2,p38z)
        call dtdpcb(p1,p2,p38z,z18z,z28z,z38z,x,y,z8z,
&      d18z,d28z,d38z,1)
        write (lud,78762) p1,p2,x,y
78755 continue
78756 continue
    do 78761 l=0,nsave0
        write (lud,78762) tout(l)
        do 78760 ieq=1,neqn
            do 78759 ider=1,3
                do 78758 i=0,np1
                    do 78757 j=0,np2
                        write (lud,78762) uout(i,j,ider,ieq,l)
78757 continue
78758 continue
78759 continue
78760 continue
78761 continue
78762 format (e16.8)
        write (lun,*) '% Read solution from pde2d.rdm'
        write (lun,*) 'NSAVE = fscanf(fid, ''%g'',1);'
        write (lun,*) 'NEQN = fscanf(fid, ''%g'',1);'
        write (lun,*) 'NP1 = fscanf(fid, ''%g'',1);'
        write (lun,*) 'NP2 = fscanf(fid, ''%g'',1);'
        if (itype.eq.2) then
            write (lun,*) 'L0 = 0;'
        else
            write (lun,*) 'L0 = 1;'
        endif
        write (lun,*) 'T = zeros(NSAVE+1,1);'
        write (lun,*) 'P1 = zeros(NP2+1,NP1+1);'
        write (lun,*) 'P2 = zeros(NP2+1,NP1+1);'
        write (lun,*) 'X = zeros(NP2+1,NP1+1);'
        write (lun,*) 'Y = zeros(NP2+1,NP1+1);'
        write (lun,*) 'U = zeros(NP2+1,NP1+1,NSAVE+1,3,NEQN);'
        write (lun,*) 'for i=0:NP1'

```

```

write (lun,*) 'for j=0:NP2'
write (lun,*) ' P1(j+1,i+1) = fscanf(fid,'%g',1);'
write (lun,*) ' P2(j+1,i+1) = fscanf(fid,'%g',1);'
write (lun,*) ' X(j+1,i+1) = fscanf(fid,'%g',1);'
write (lun,*) ' Y(j+1,i+1) = fscanf(fid,'%g',1);'
write (lun,*) 'end'
write (lun,*) 'end'
write (lun,*) 'for l=0:NSAVE'
write (lun,*) 'T(l+1) = fscanf(fid,'%g',1);'
write (lun,*) 'for ieq=1:NEQN'
write (lun,*) 'for ider=1:3'
write (lun,*) 'for i=0:NP1'
write (lun,*) 'for j=0:NP2'
write (lun,*)
& ' U(j+1,i+1,l+1,ider,ieq) = fscanf(fid,'%g',1);'
write (lun,*) 'end'
write (lun,*) 'end'
write (lun,*) 'end'
write (lun,*) 'end'
write (lun,*) 'end'
write (lun,*) 'xmin = min(min(X(:,:)));'
write (lun,*) 'xmax = max(max(X(:,:)));'
write (lun,*) 'ymin = min(min(Y(:,:)));'
write (lun,*) 'ymax = max(max(Y(:,:)));'
write (lun,*) 'hx = 0.1*(xmax-xmin);'
write (lun,*) 'hy = 0.1*(ymax-ymin);'
write (lun,*) '% Surface plots of each variable'
write (lun,*) 'for IEQ=1:NEQN'
write (lun,*) 'IDER = 1;'
write (lun,*)
& 'umin = min(min(min(U(:,: ,L0+1:NSAVE+1, IDER, IEQ))));'
write (lun,*)
& 'umax = max(max(max(U(:,: ,L0+1:NSAVE+1, IDER, IEQ))));'
write (lun,*) 'for L=L0:NSAVE'

write (lun,*) ' surf(X,Y,U(:,: ,L+1, IDER, IEQ))'
write (lun,*) ' colorbar'
write (lun,*) ' axis([xmin xmax ymin ymax umin umax])'
write (lun,*) ' xlabel(''X'')'
write (lun,*) ' ylabel(''Y'')'
write (lun,*) ' zlabel([''U'',num2str(IEQ)])'
write (lun,*) ' title(['' T = '',num2str(T(L+1))])'
write (lun,*) ' view(50,40.0)'
write (lun,*) ' caxis([0.1 0.3])'
write (lun,*) ' saveas(gcf,[''wave'',num2str(L),''.jpg'']);'
write (lun,*) 'end'
write (lun,*) 'end'

return
end

```